Fast Quantum Algorithm for Differential Equations

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arXiv:2306.11802 (2023)
Fast quantum algorithm for differential equations

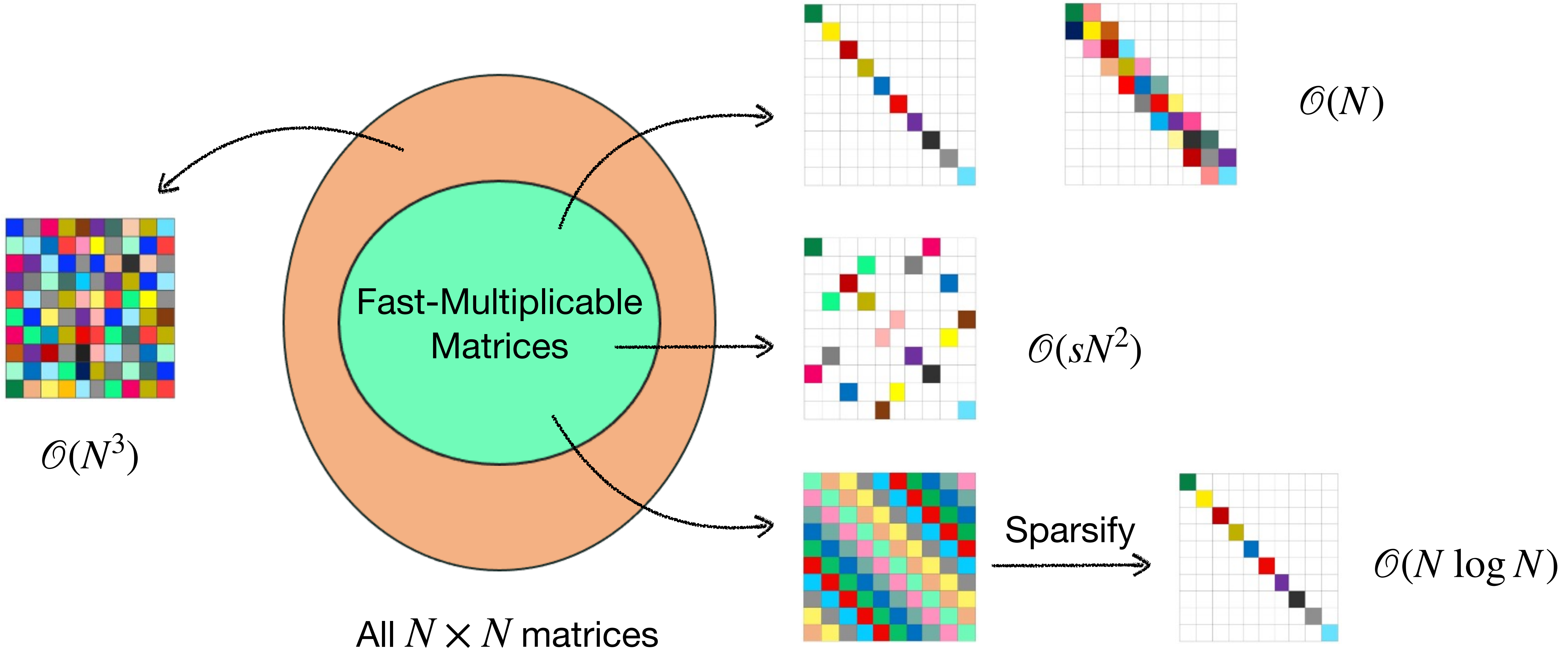
arXiv:2309.09350 (2023)
Efficient quantum algorithm for all quantum wavelet transforms

Toronto

Toronto in Winter!

Context: Generic vs Structured Problems

Matrix multiplication



Timeline of matrix multiplication exponent

Year	Bound on omega	Authors
1969	2.8074	Strassen[1]
1978	2.796	Pan[11]
1979	2.780	Bini, Capovani, Romani[12]
1981	2.522	Schönhage[13]
1981	2.517	Romani[14]
1981	2.496	Coppersmith, Winograd[15]
1986	2.479	Strassen[16]
1990	2.3755	Coppersmith, Winograd[17]
2010	2.3737	Stothers[18]
2013	2.3729	Williams[19][20]
2014	2.3728639	Le
2020	2.3728596	Aln
2022	2.37188	Du

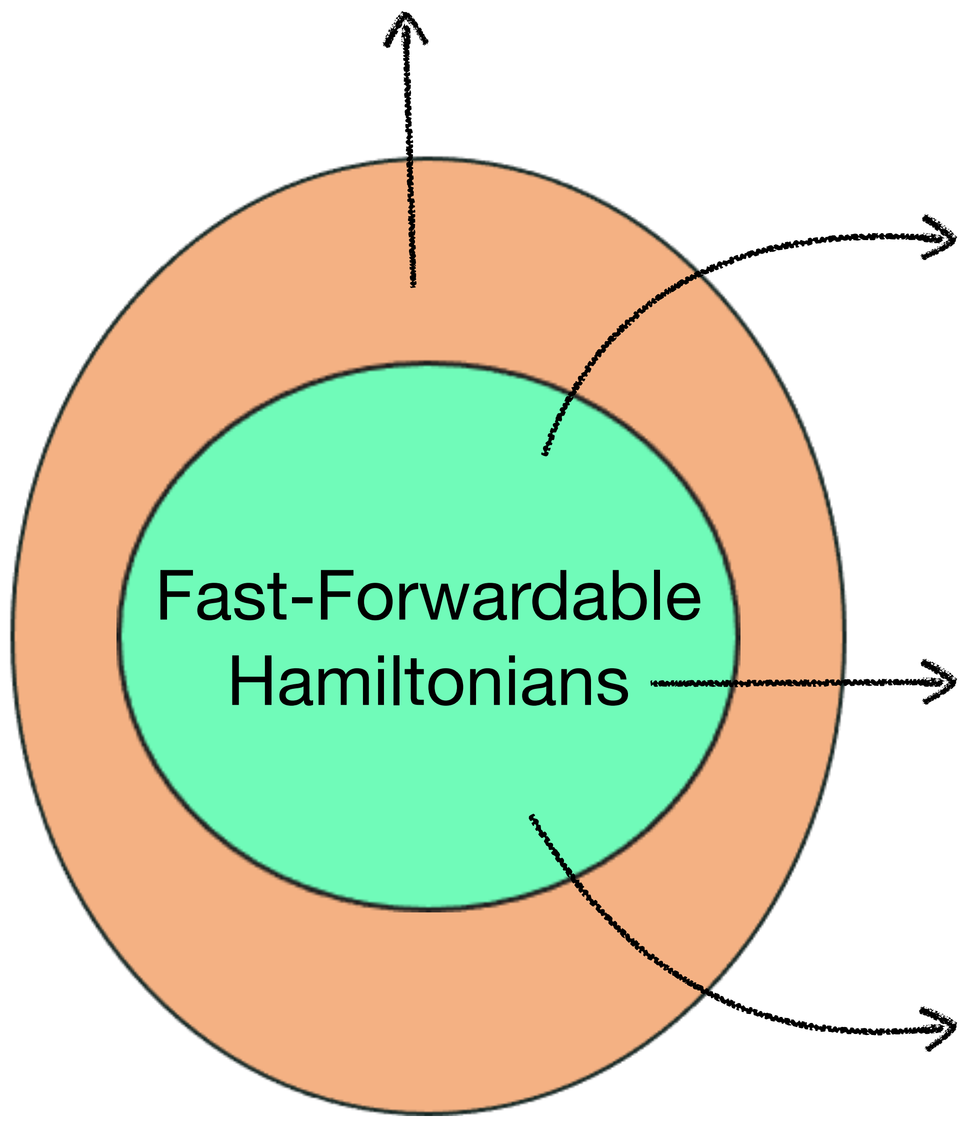
Galactic Algorithms

No-go: $\Omega(N^2)$

Context: Generic vs Structured Problems

Hamiltonian simulation: e^{-iHt}

No fast-forwarding theorem: [Berry, Ahokes, Cleve, Sanders `07]
no sublinear-in-t simulation algorithm



All Hamiltonians

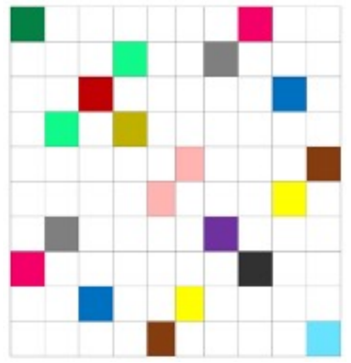
Efficiently diagonalizable Hamiltonians $e^{-iHt} = Ue^{-iDt}U^\dagger$

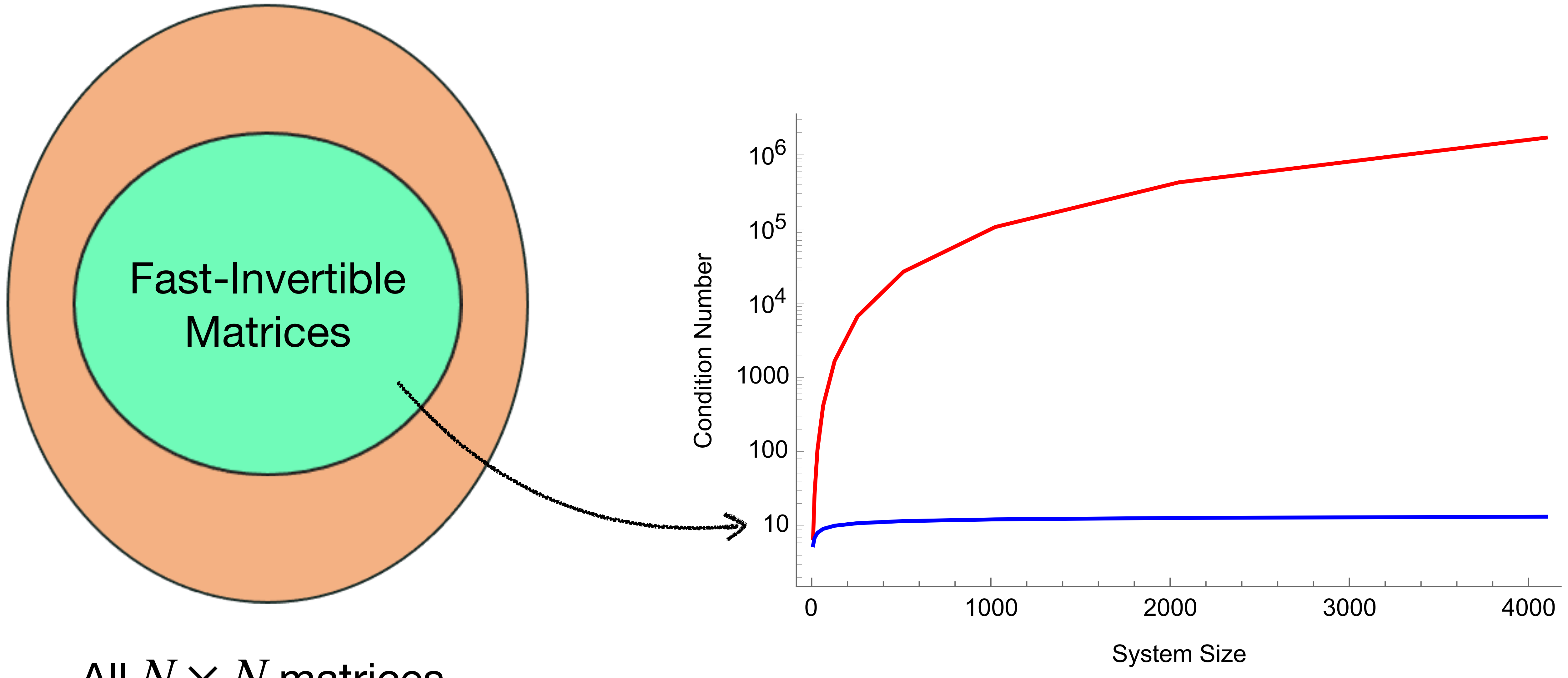
Commuting local Hamiltonians $e^{-iHt} = \Pi_j e^{-iH_j t}$ [Atia, Aharonov`17]

Hamiltonians with integer spectra $e^{-iHt} = e^{-iH(t \bmod 2\pi)}$

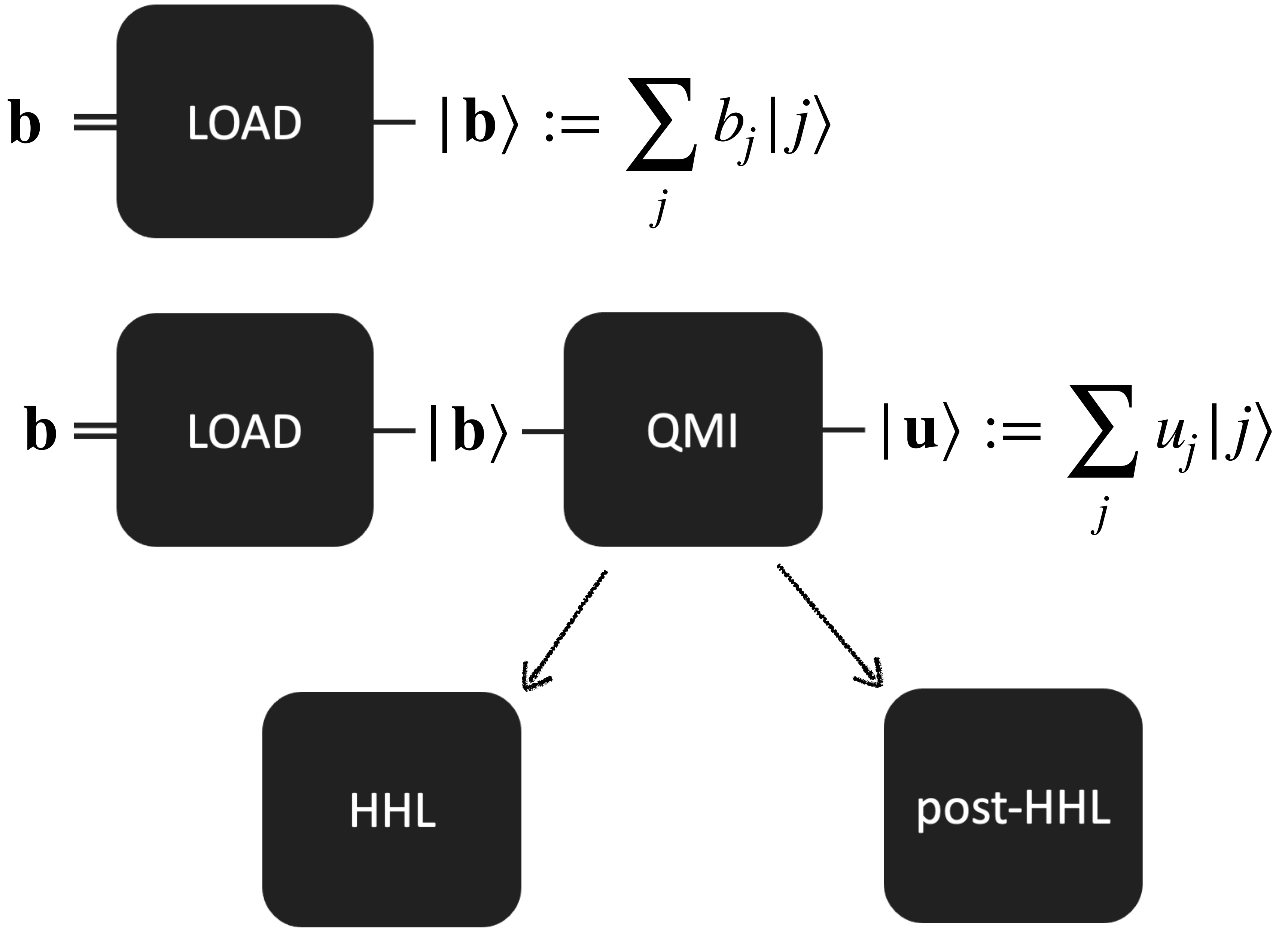
Context: Generic vs Structured Problems

Linear system of equations: $A\mathbf{u} = \mathbf{b}$





All $N \times N$ matrices



[Harrow, Hassidim, Lloyd `09]

$\tilde{\mathcal{O}}(\log(N) s^2 \kappa^2 / \varepsilon)$

[Childs, Kothari, Somma `15]
[Gilyen, Su, Low, Wiebe `19]

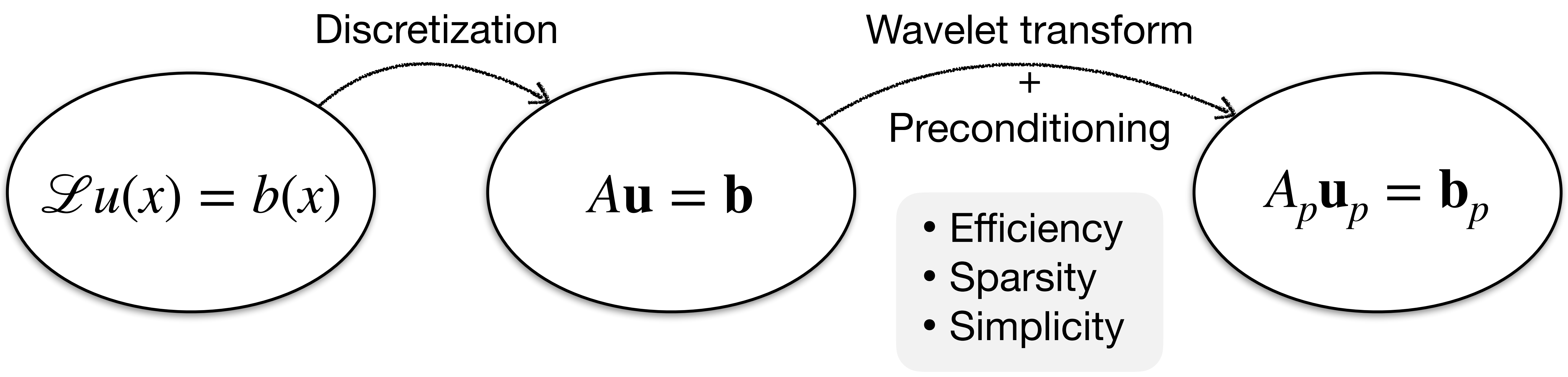
$\tilde{\mathcal{O}}(\kappa \log(\kappa / \varepsilon))$

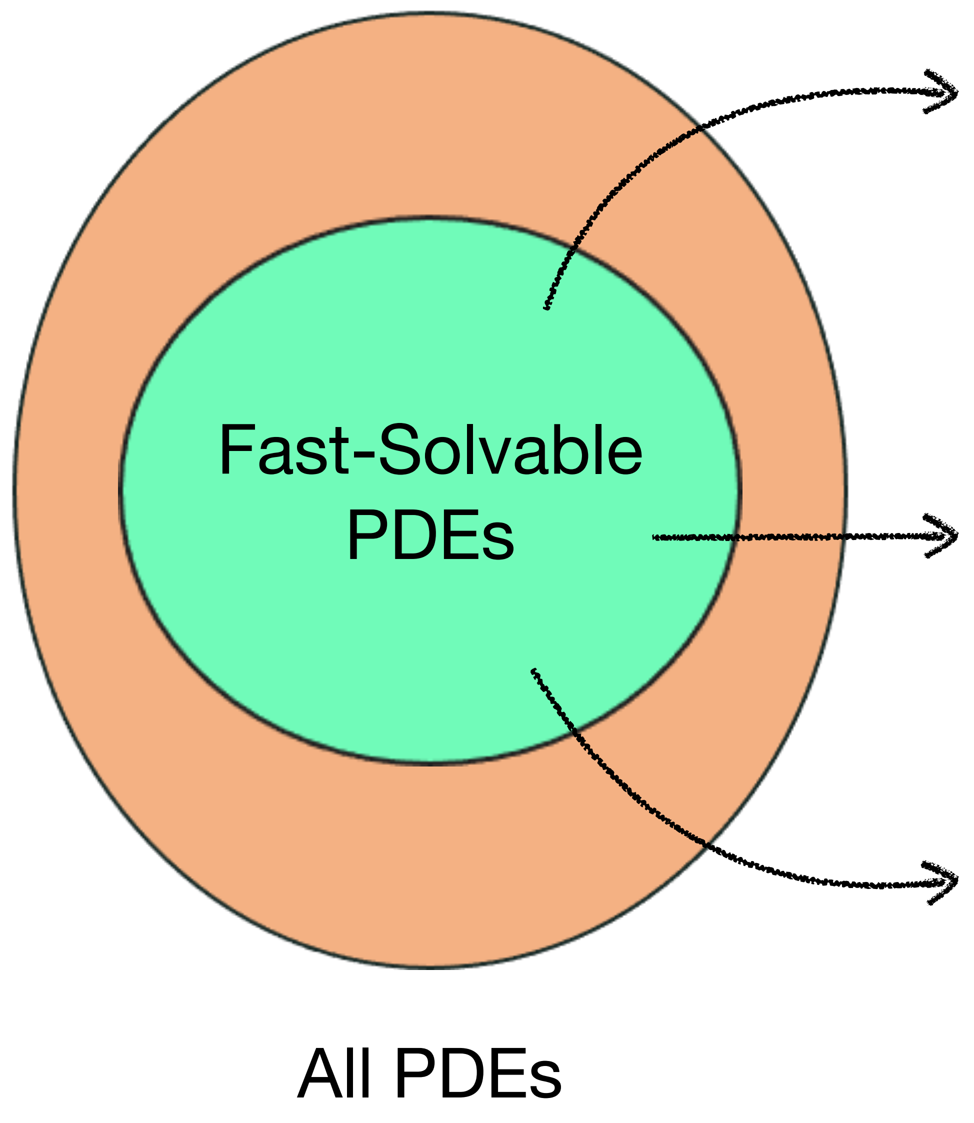
No-go: $\mathcal{O}(\kappa \log(1/\varepsilon))$

[Costa, An, Sanders, et al. `22]

Classical: conjugate gradient method; $\mathcal{O}(N s \kappa \log(1/\varepsilon))$

Context: Generic vs Structured Problems





Constant-coefficient 2nd order linear PDEs

$$\frac{\mathrm{d}^2}{\mathrm{d}x^2} - \frac{\mathrm{d}}{\mathrm{d}x} + \mathbb{I}$$

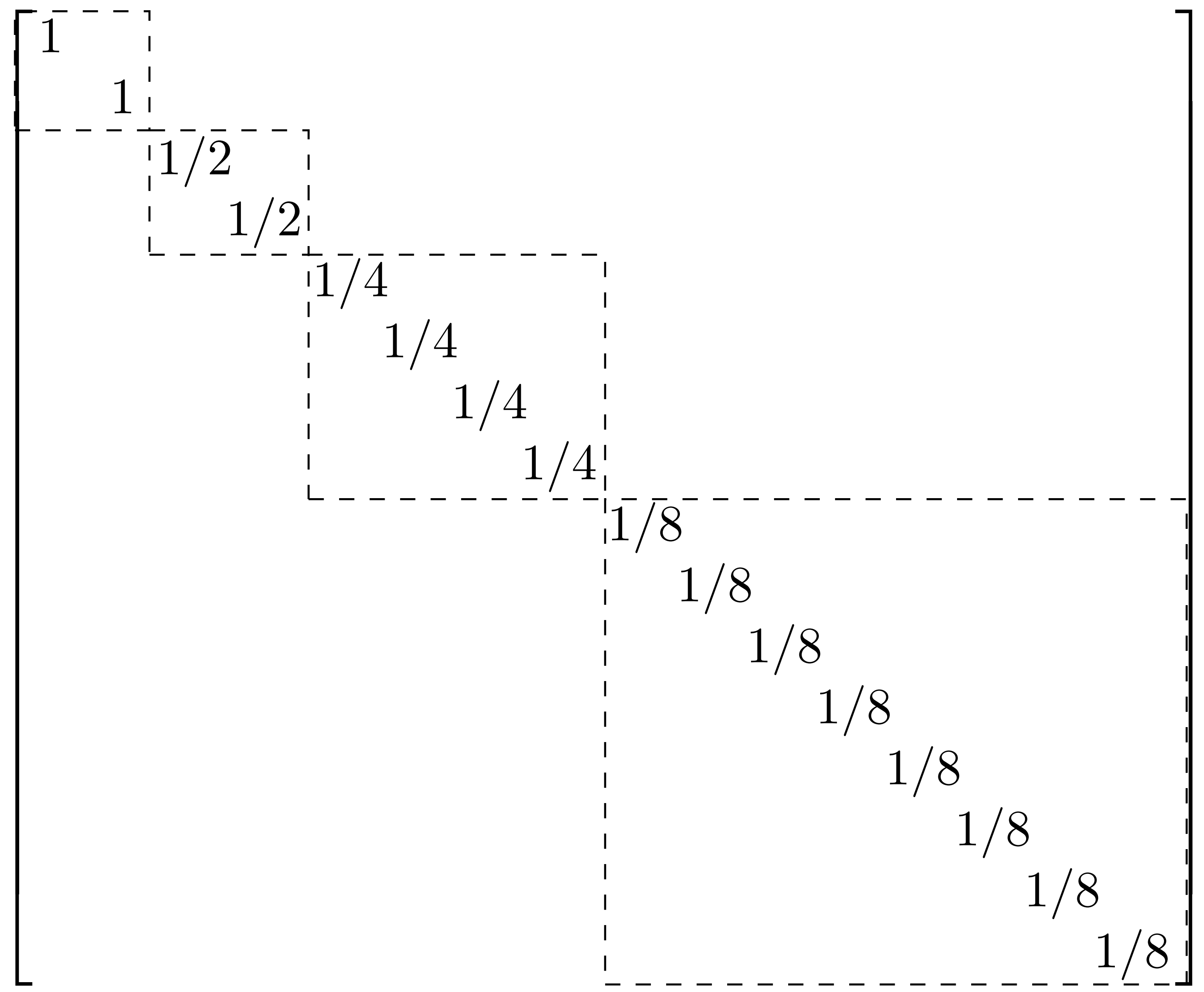
Slowly-varying-coefficient 2nd order PDEs

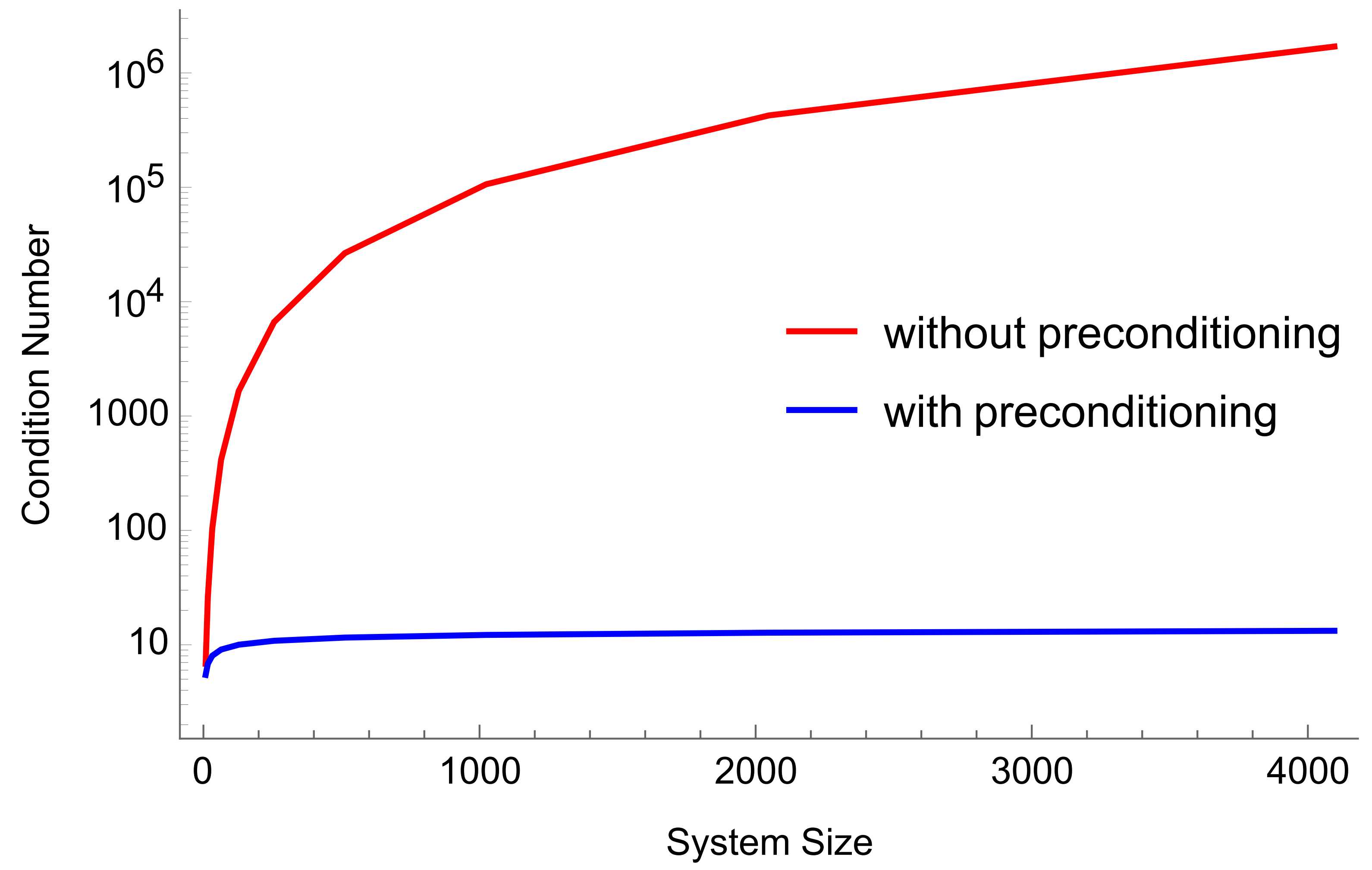
$$-\frac{\mathrm{d}}{\mathrm{d}x}\left(\cosh\left(\frac{x}{4}\right)\frac{\mathrm{d}}{\mathrm{d}x}\right) + \mathrm{e}^x\mathbb{I}$$

Higher-order PDEs

$$\frac{\mathrm{d}^4}{\mathrm{d}x^4}$$

With mild conditions!



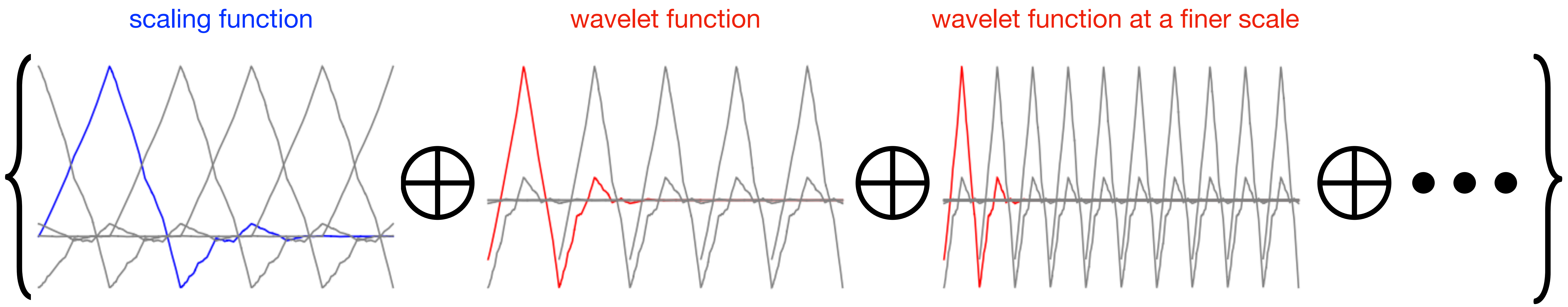


The Rest

- Wavelet bases, transformation, and preconditioning
- Fast-solvable differential equations
- The algorithm and its complexity

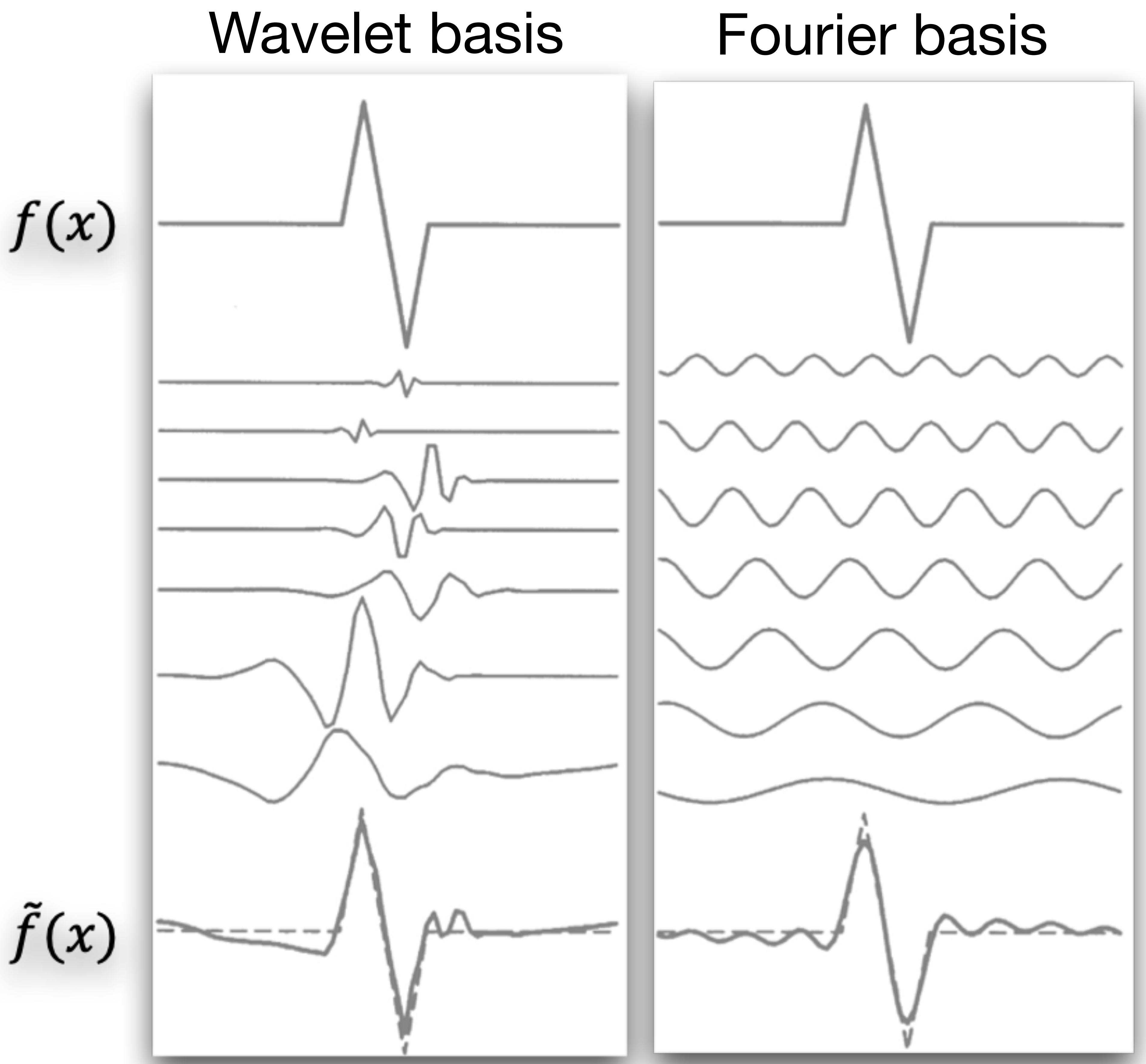
Wavelet basis

$L^2(\mathbb{R}) = \text{Span}$



- Locality in real and dual spaces
- Differentiability
- Sparse representations
  - Compression
  - Faster algorithms
- Efficient preconditioning

  [Bagherimehrab, Nakaji, Wiebe, Aspuru-Guzik `23]



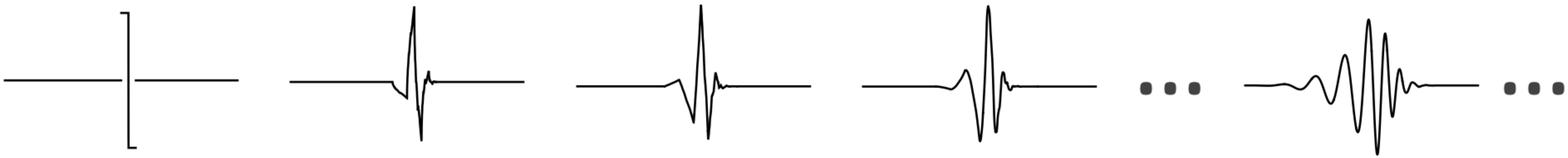
Wavelets zoo

Daubechies | Coiflet | Symlet | CDF 5/3 | CDF 9/7

and many more!

Daubechies family

Index = 1 | Index = 2 | Index = 3 | Index = 4 | Index = 12

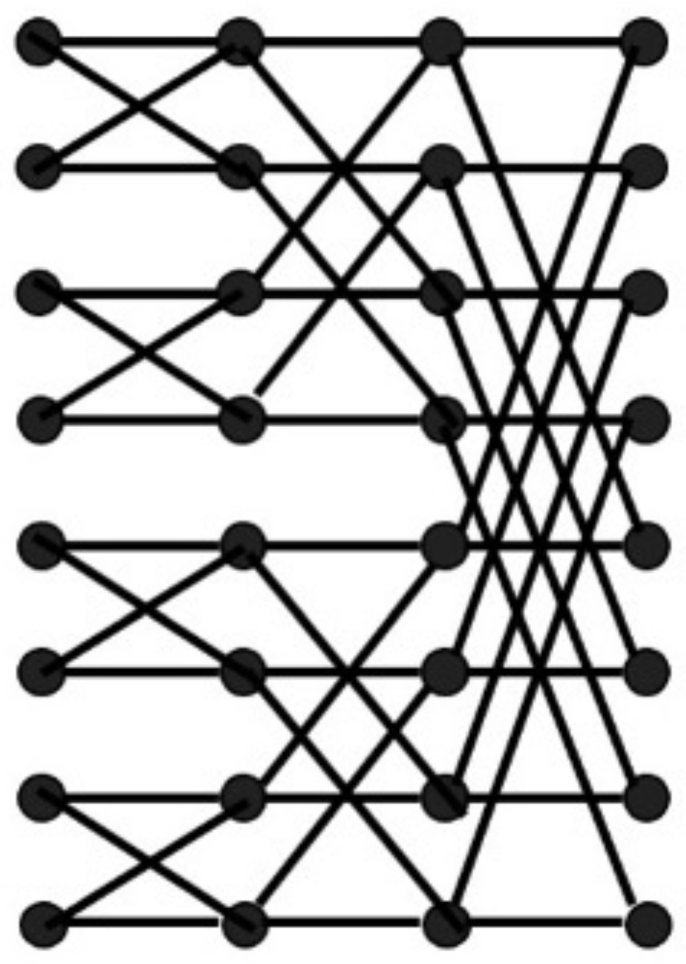


$[h_0, h_1]$ | $[h_0, h_1, h_2, h_3]$ | $[h_0, h_1, h_2, h_3, h_4, h_5]$ | $[h_0, h_1, h_2, h_3, h_4, h_5, h_6, h_7]$

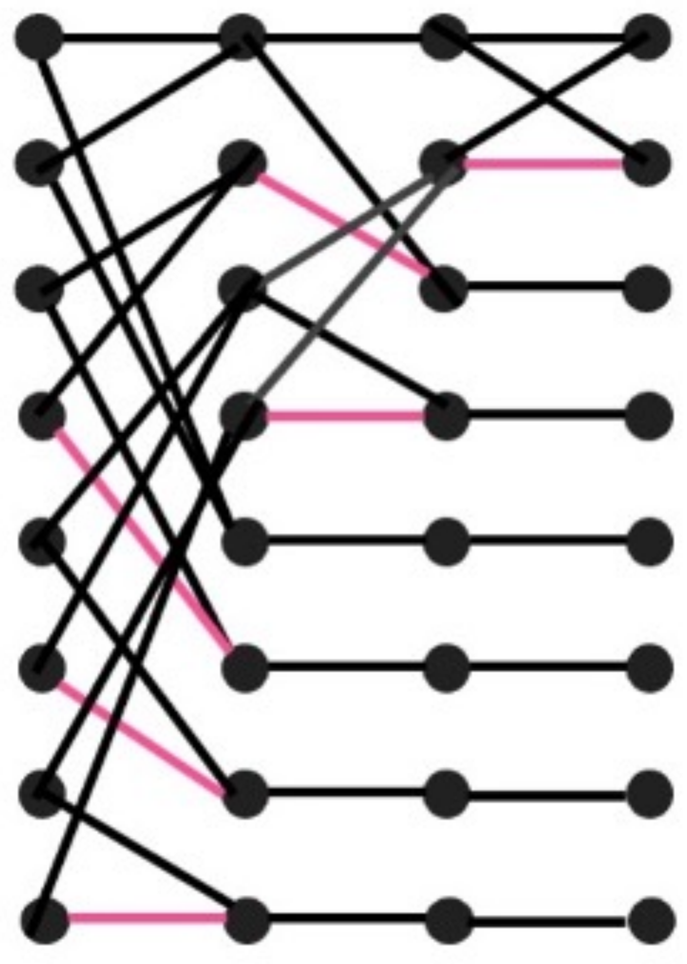
Specified by a sequence of numbers

Fourier vs wavelet transform

FFT

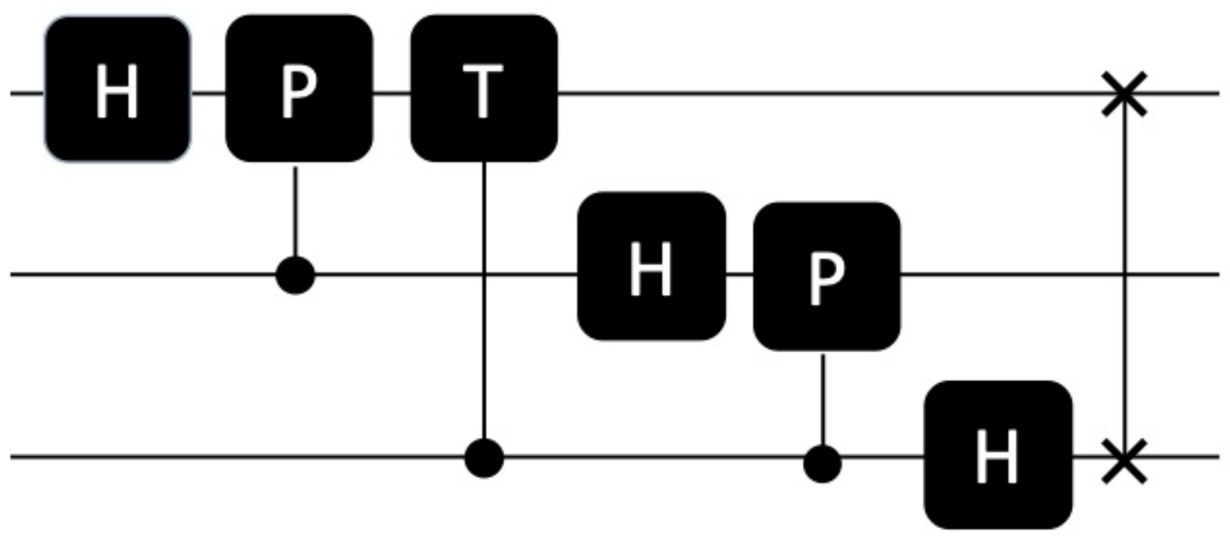


FWT

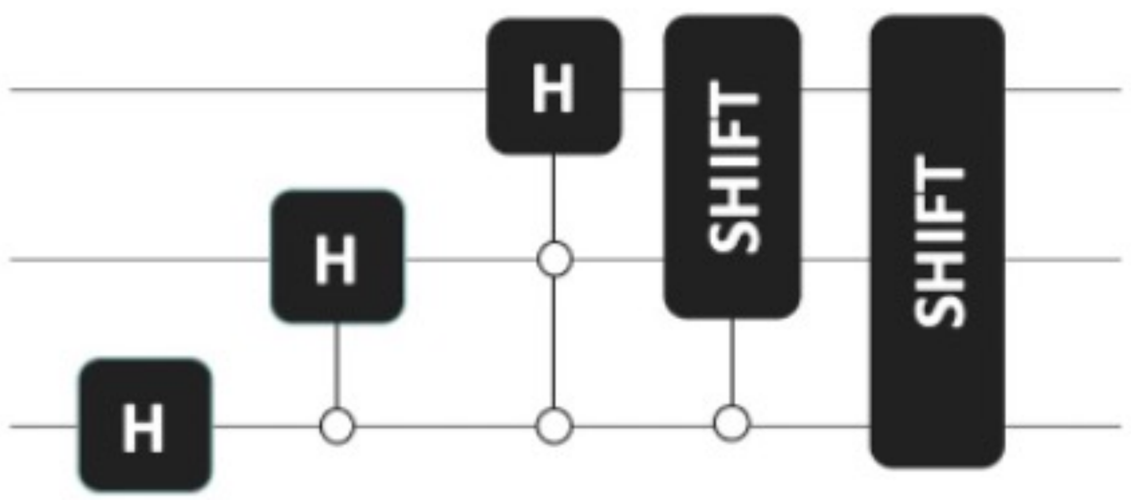


$$\mathcal{O}(N \log N)$$

QFT



QWT

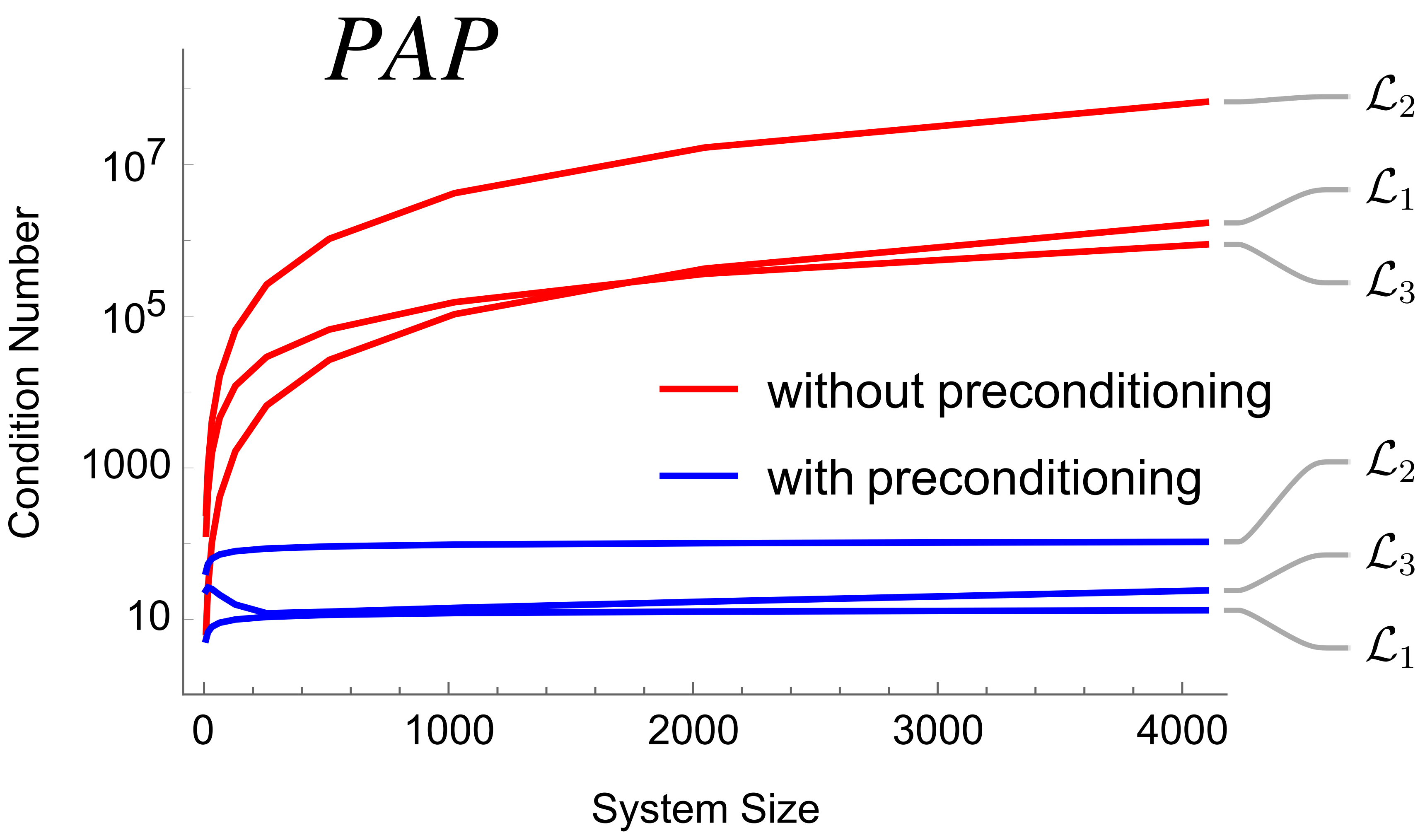


$$\mathcal{O}(n^2)$$

$$n = \log N$$

[Bagherimehrab, Aspuru-Guzik `23]

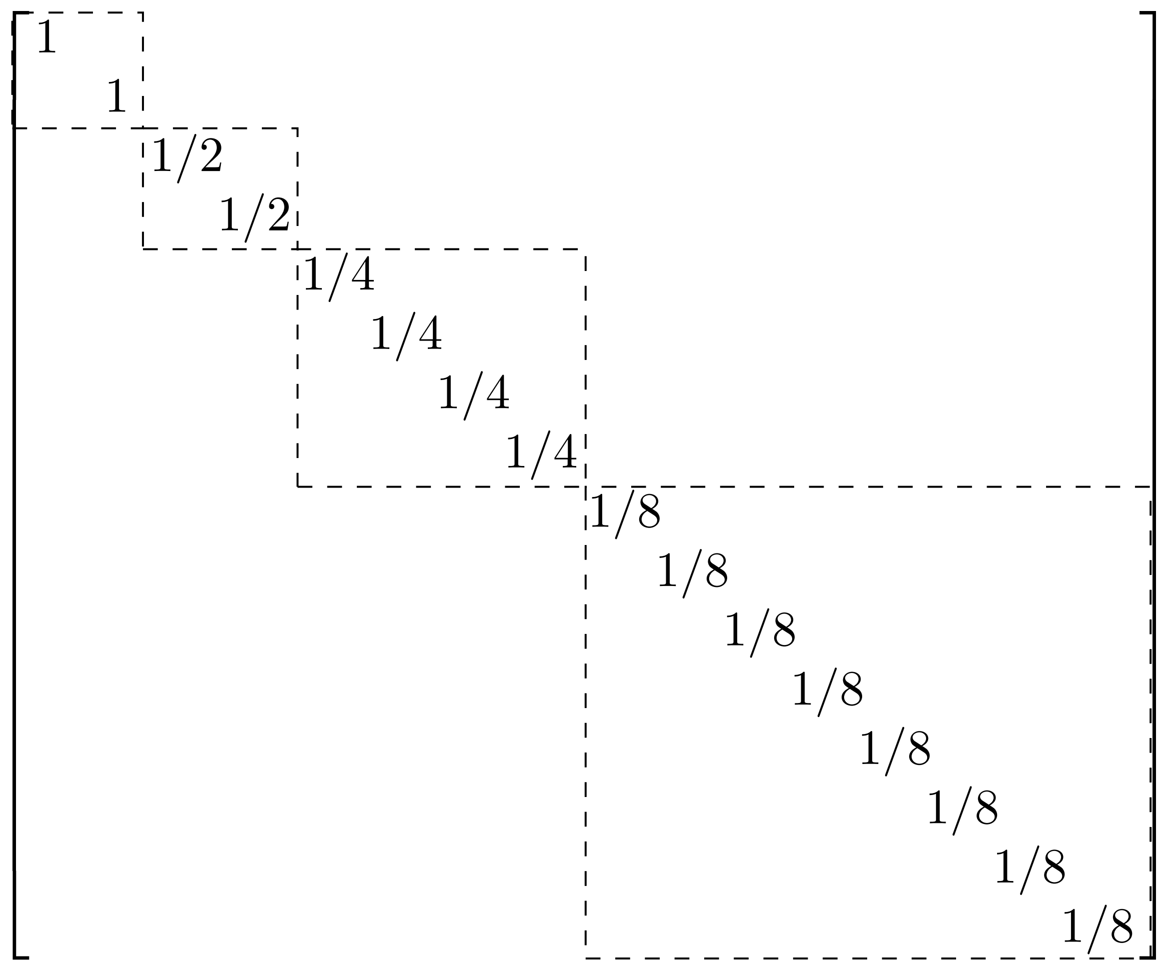
Wavelet Preconditioning



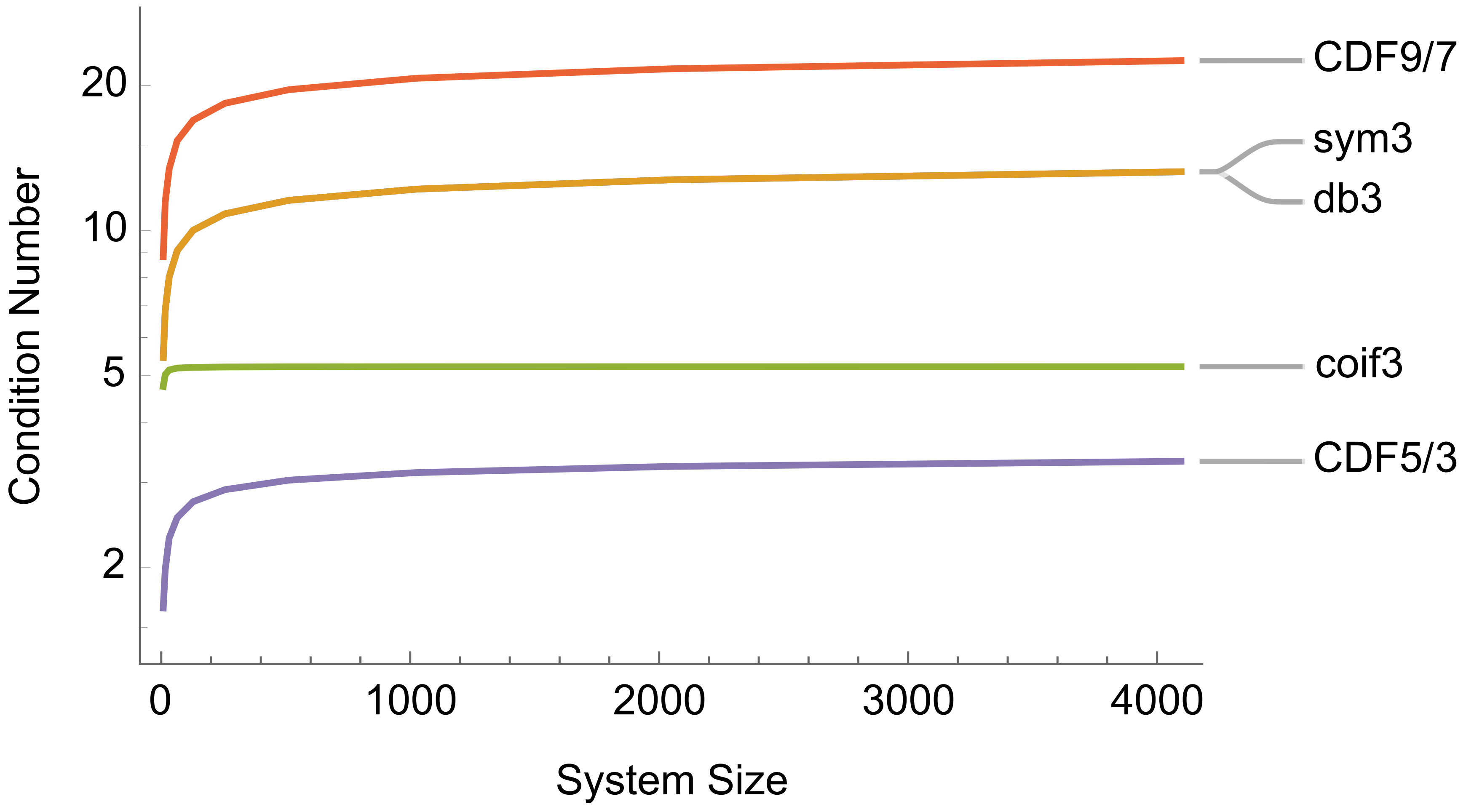
$$\mathcal{L}_1 := \frac{d^2}{dx^2}$$

$$\mathcal{L}_2 := \frac{d^2}{dx^2} - \frac{d}{dx} + \mathbb{I}$$

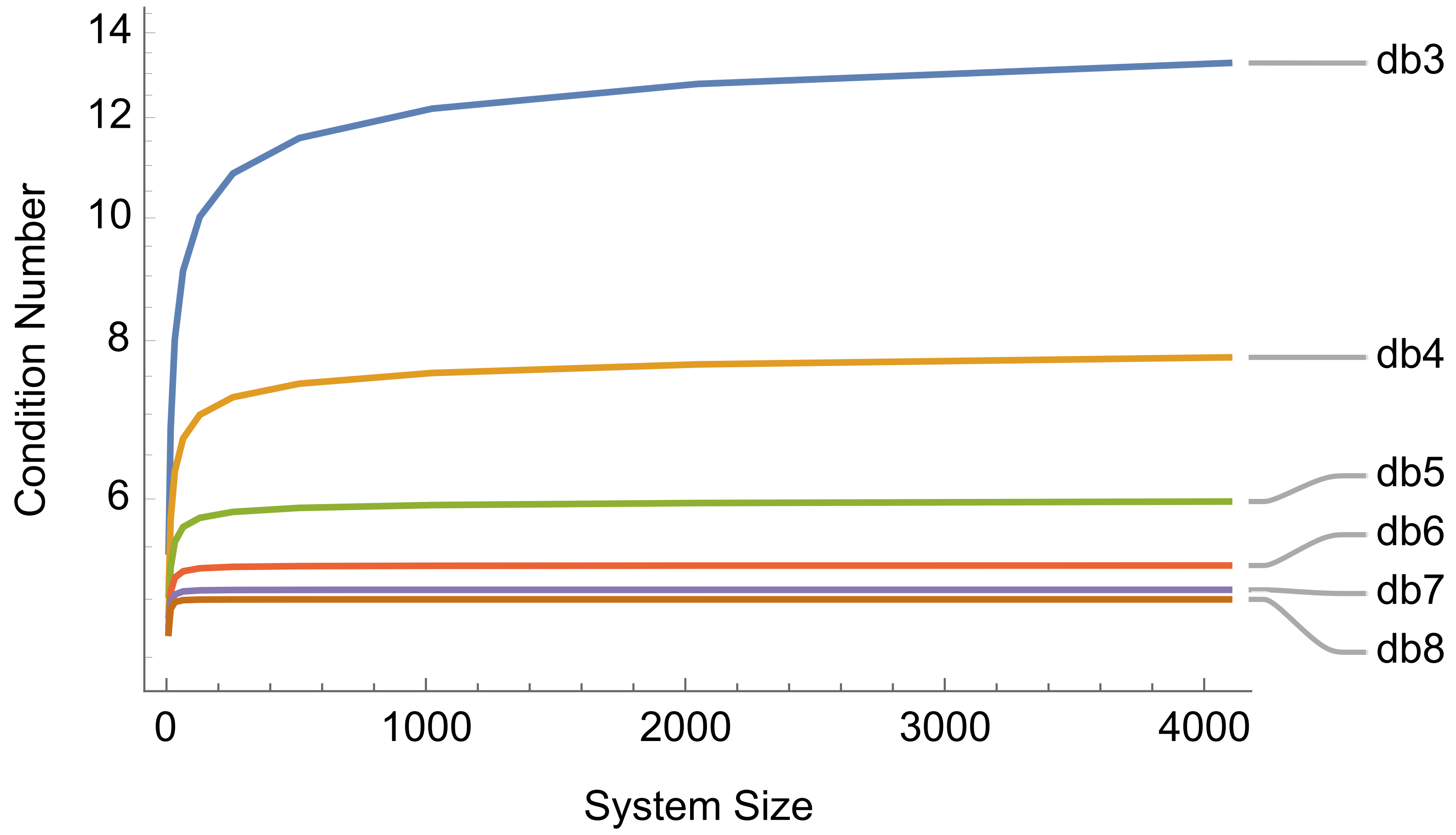
$$\mathcal{L}_3 := -\frac{d}{dx}\left(\cosh\left(\frac{x}{4}\right)\frac{d}{dx}\right) + e^x\mathbb{I}$$



Structured diagonal matrix



$$\mathcal{L}_1 := \frac{d^2}{dx^2}$$



Fast-Solvable Differential Equations

ODEs (for simplicity)

$$\mathcal{L}u(x) = b(x)$$

$$\mathcal{L}u(x) = \sum_{s=0}^{m} c_s(x) \frac{\mathrm{d}^s}{\mathrm{d}x^s} u(x)$$

$$B(u,v) = \int u(x) \mathcal{L}v(x) \, \mathrm{d}x$$

- Symmetric: $B(u,v) = B(v,u)$
- Bounded: $B(u,v) \leq C\|u\|\|v\|$
- Coercive (or elliptic): $B(u,u) \geq c\|u\|^2$

$$0 < c < C$$

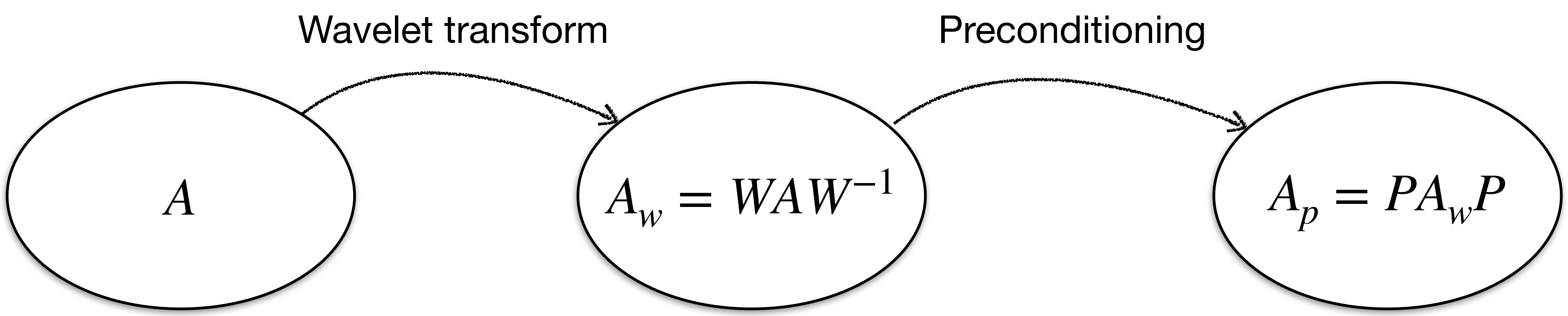
Sturm-Liouville Problems

$$\mathcal{L}_{\mathrm{ST}} = -\frac{\mathrm{d}}{\mathrm{d}x}\left(p(x)\frac{\mathrm{d}}{\mathrm{d}x}\right) + q(x)$$

$$C_1 \leq p(x) \leq C_2 \qquad 0 \leq q(x) \leq C_3$$

- Poisson equation
  $p(x) = 1, \qquad q(x) = 0$
- 1D time-independent Schrödinger equation
  $p(x) = 1, \qquad q(x) = V(x)$
- Helmholtz
  $p(x) = 1, \qquad q(x) = C$

Algorithm and Complexity



$A|\mathbf{u}\rangle = |\mathbf{b}\rangle$ $\qquad$ $WAW^{-1}W|\mathbf{u}\rangle = W|\mathbf{b}\rangle$ $\qquad$ $PA_wPP^{-1}W|\mathbf{u}\rangle = PW|\mathbf{b}\rangle$

$$P = \frac{1}{2}(U^+ + U^-) \qquad U^{\pm} := P \pm i\sqrt{\mathbb{I} - P^2}$$

$$|\mathbf{u}\rangle = W^{-1}PA_p^{-1}PW|\mathbf{b}\rangle$$

$$= \frac{1}{4}\sum_{a,b} W^{-1}U^aA_p^{-1}U^bW|\mathbf{b}\rangle$$

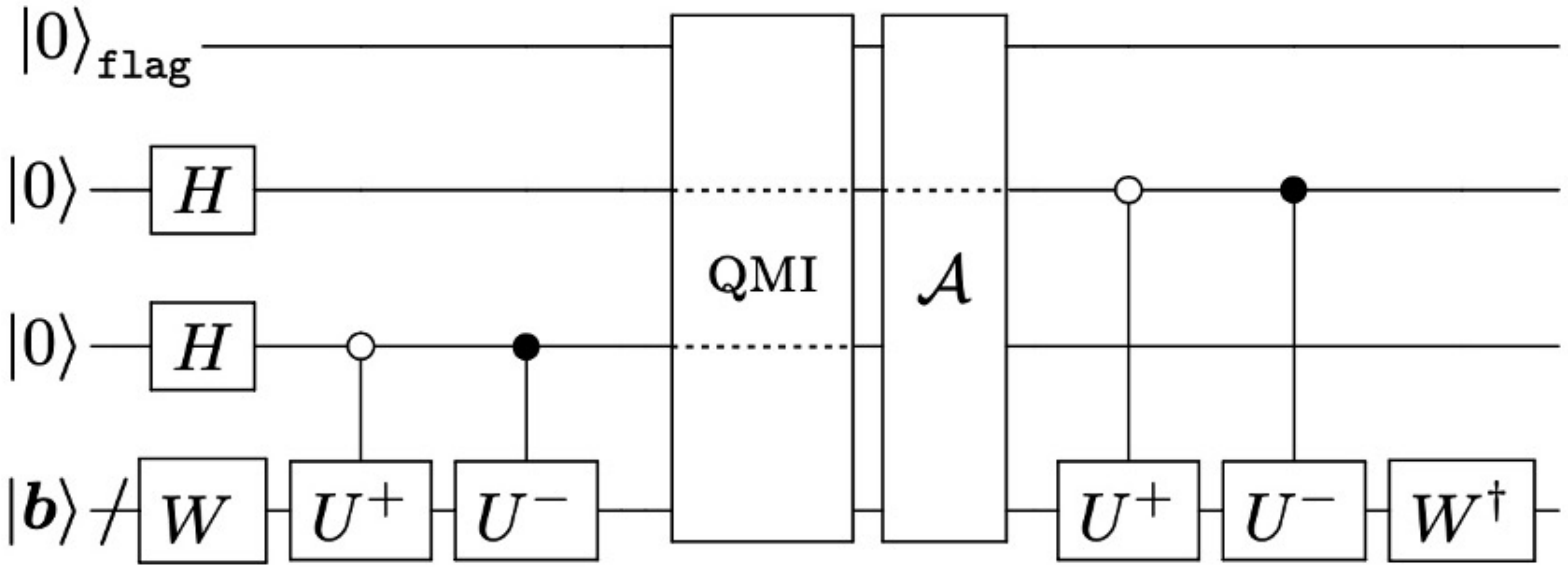
$$\begin{bmatrix} 1 &&&&&&&&&&&&&& \\ & 1 &&&&&&&&&&&&& \\ && 1/2 &&&&&&&&&&&& \\ &&& 1/2 &&&&&&&&&&& \\ &&&& 1/4 &&&&&&&&&& \\ &&&&& 1/4 &&&&&&&&& \\ &&&&&& 1/4 &&&&&&&& \\ &&&&&&& 1/4 &&&&&&& \\ &&&&&&&& 1/8 &&&&&& \\ &&&&&&&&& 1/8 &&&&& \\ &&&&&&&&&& 1/8 &&&& \\ &&&&&&&&&&& 1/8 &&& \\ &&&&&&&&&&&& 1/8 && \\ &&&&&&&&&&&&& 1/8 & \\ &&&&&&&&&&&&&& 1/8 \\ &&&&&&&&&&&&&&& 1/8 \end{bmatrix}$$

$$\begin{bmatrix} 1 &&&&&&&&&&&&&& \\ & 1 &&&&&&&&&&&&& \\ && e^{\pm i\theta_1} &&&&&&&&&&&& \\ &&& e^{\pm i\theta_1} &&&&&&&&&&& \\ &&&& e^{\pm i\theta_2} &&&&&&&&&& \\ &&&&& e^{\pm i\theta_2} &&&&&&&&& \\ &&&&&& e^{\pm i\theta_2} &&&&&&&& \\ &&&&&&& e^{\pm i\theta_2} &&&&&&& \\ &&&&&&&& e^{\pm i\theta_3} &&&&&& \\ &&&&&&&&& e^{\pm i\theta_3} &&&&& \\ &&&&&&&&&& e^{\pm i\theta_3} &&&& \\ &&&&&&&&&&& e^{\pm i\theta_3} &&& \\ &&&&&&&&&&&& e^{\pm i\theta_3} && \\ &&&&&&&&&&&&& e^{\pm i\theta_3} & \\ &&&&&&&&&&&&&& e^{\pm i\theta_3} \\ &&&&&&&&&&&&&&& e^{\pm i\theta_3} \end{bmatrix}$$

Algorithm and Complexity

$$|\mathbf{u}\rangle = \frac{1}{4}\sum_{a,b} W^{-1}U^a A_p^{-1} U^b W|\mathbf{b}\rangle$$

$|\psi_{ab}\rangle$



$$\langle \mathbf{u}|M|\mathbf{u}\rangle = \frac{1}{16}\sum_{abcd}\langle\psi_{ab}|M|\psi_{cd}\rangle$$

$$|\psi\rangle := \frac{1}{2}\sum_{a,b}|ab\rangle|\psi_{ab}\rangle$$

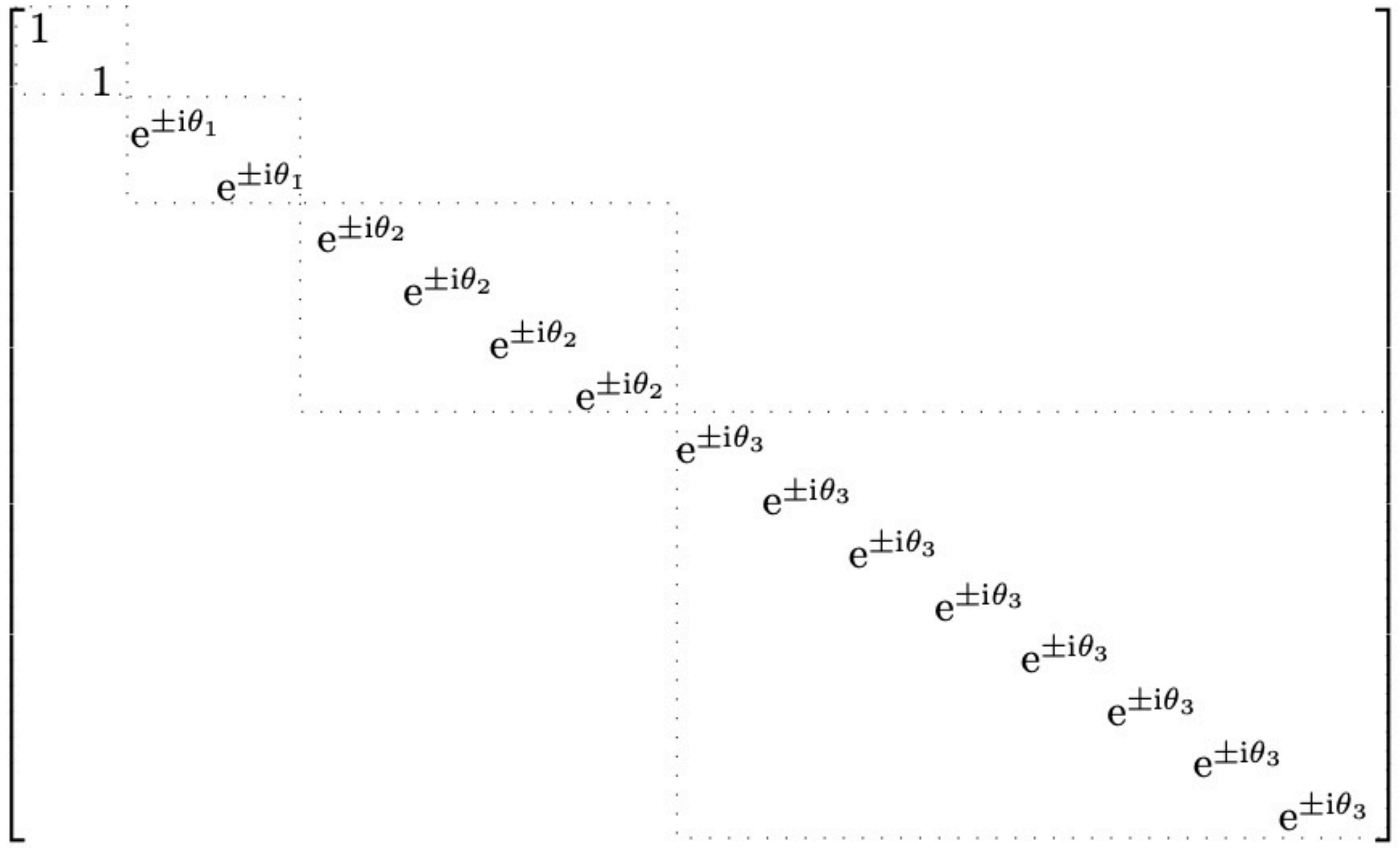
$$\langle\psi|M'|\psi\rangle = 4\langle\mathbf{u}|M|\mathbf{u}\rangle$$

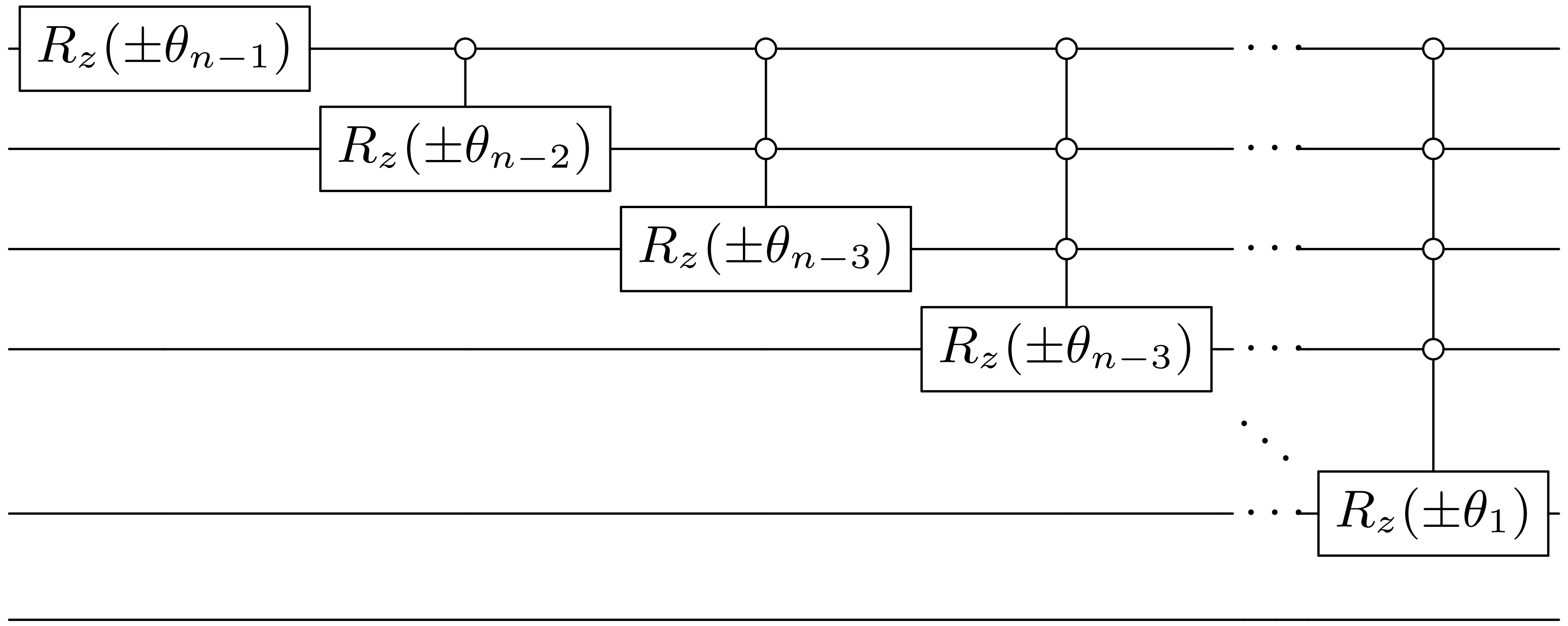
$$M' = \begin{bmatrix} M & M & M & M \\ M & M & M & M \\ M & M & M & M \\ M & M & M & M \end{bmatrix}$$

Specification: efficiently computable

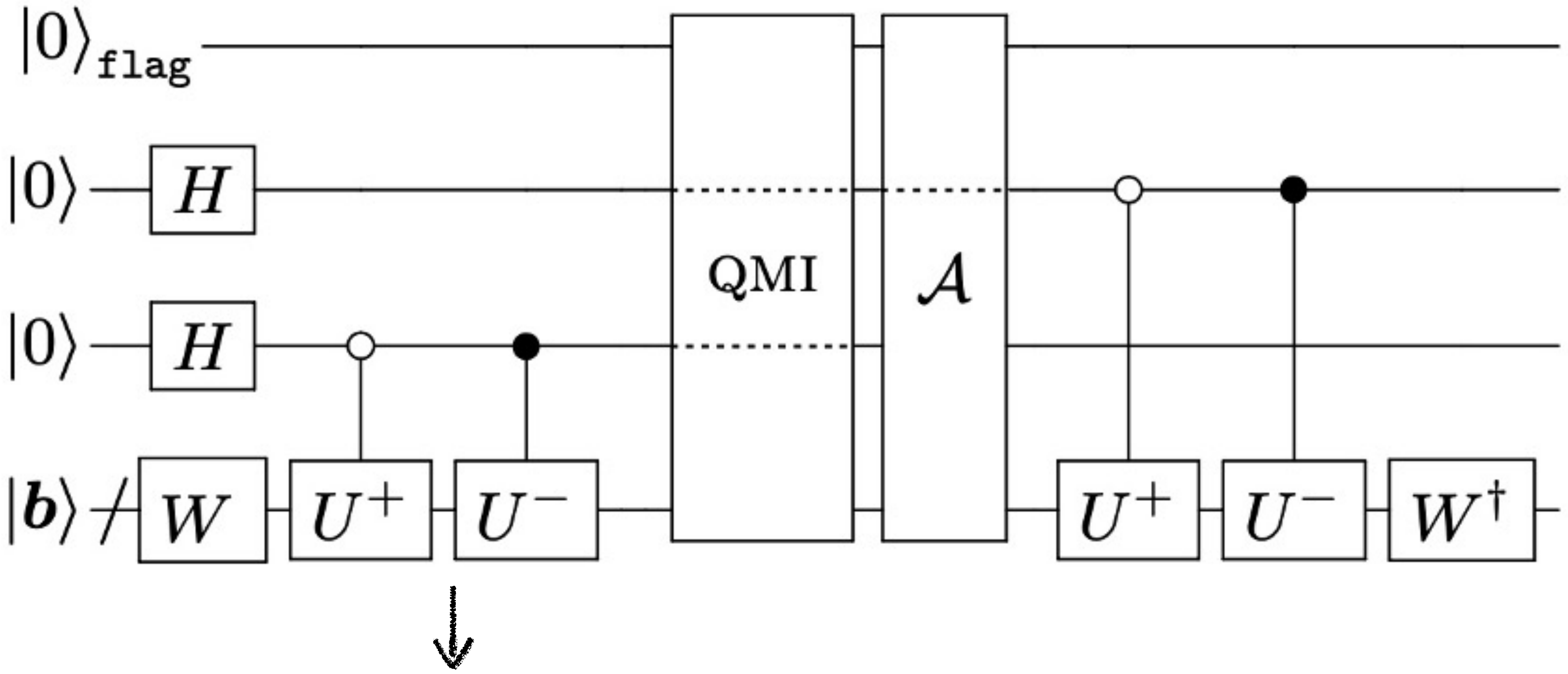
Algorithm and Complexity

$$U^{\pm} := P \pm i\sqrt{\mathbb{I} - P^2}$$





Angles: classically precomputed



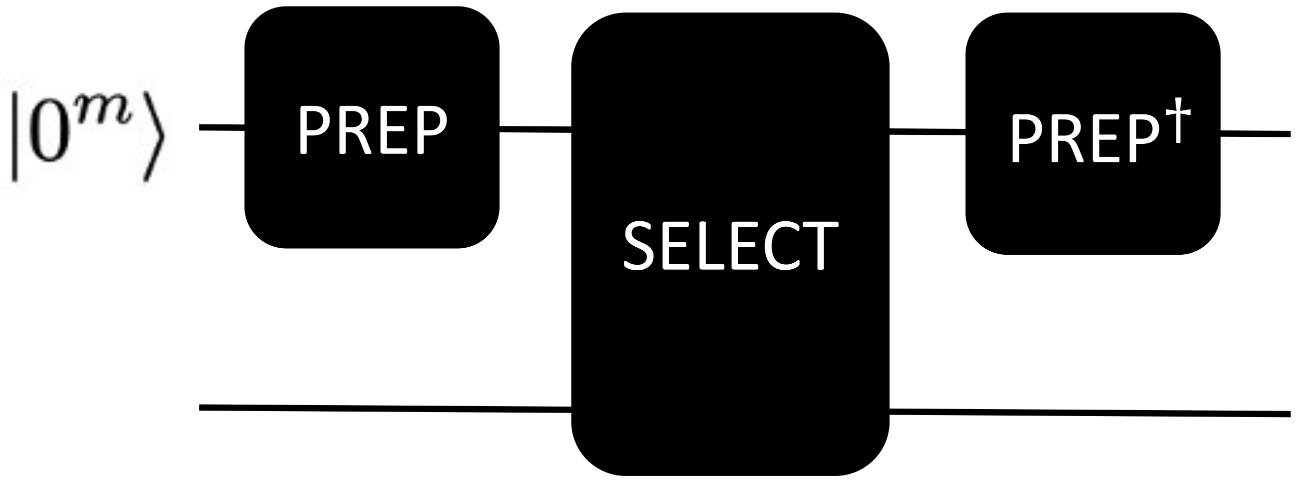
$\mathcal{O}(n)$

Gate cost

Algorithm and Complexity

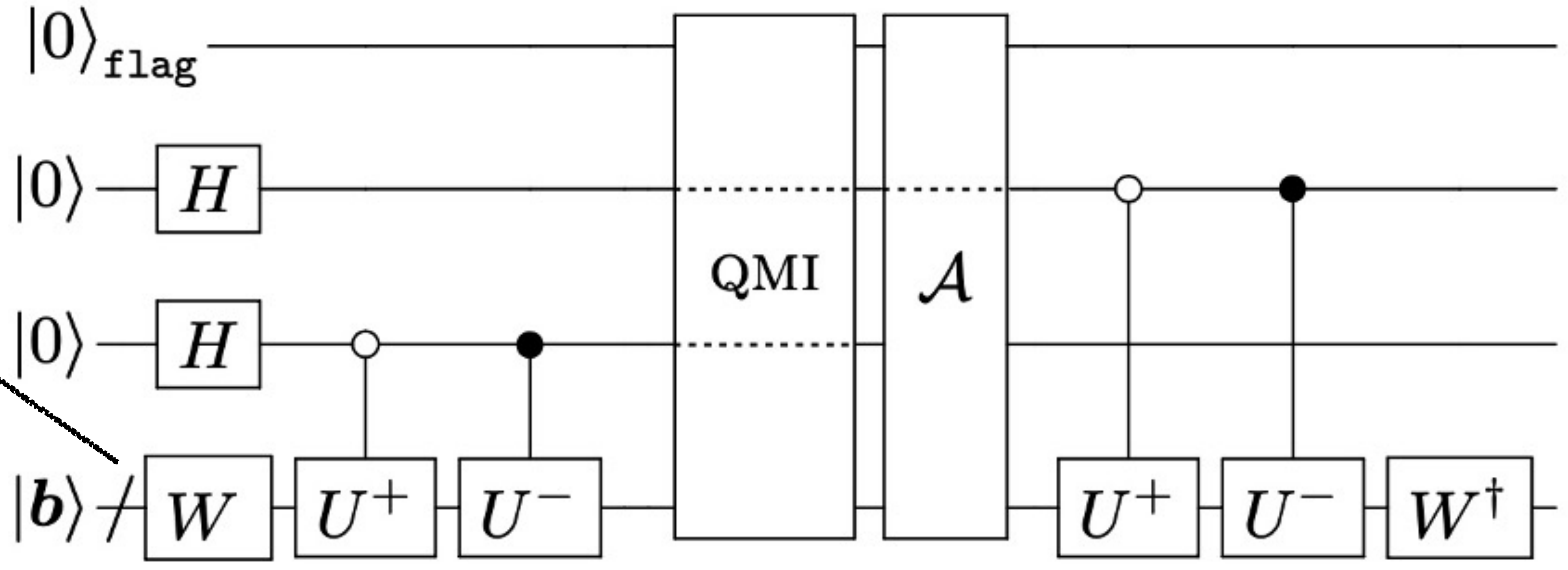
$$U = \sum_{\ell=0}^{M-1} h_\ell U_\ell, \quad U_\ell := \begin{cases} P_\ell & \text{if } \ell \text{ is odd,} \\ (Z \otimes \mathbb{1}_{n-1}) P_\ell & \text{if } \ell \text{ is even,} \end{cases}$$

$$P_\ell : |j\rangle \mapsto \begin{cases} \left|\frac{j-\ell \bmod N}{2}\right\rangle & \text{if } j \text{ and } \ell \text{ have same parity,} \\ \left|\frac{N}{2} + \frac{j+\ell-1 \bmod N}{2}\right\rangle & \text{if } j \text{ and } \ell \text{ have opposite parity.} \end{cases}$$



$$\frac{1}{\sqrt{2}} |0^m\rangle U |\psi\rangle + \frac{1}{\sqrt{2}} |\perp\rangle$$

$$\mathbf{PREP}\, |0^m\rangle := \frac{1}{\sqrt[4]{2}} \sum_{\ell=0}^{M-1} \sqrt{h_\ell}\, |\ell\rangle \qquad \mathbf{SELECT}\, |\ell\rangle\, |j\rangle := |\ell\rangle\, U_\ell\, |j\rangle$$



$\mathcal{O}(n^2)$ $\mathcal{O}(n)$ $\mathcal{O}(\kappa \log(\kappa/\varepsilon)) \rightarrow \mathcal{O}(\log(1/\varepsilon))$

Gate cost

Query cost

$\mathcal{O}(1)$

Query cost

[Bagherimehrab, Aspuru-Guzik `23]

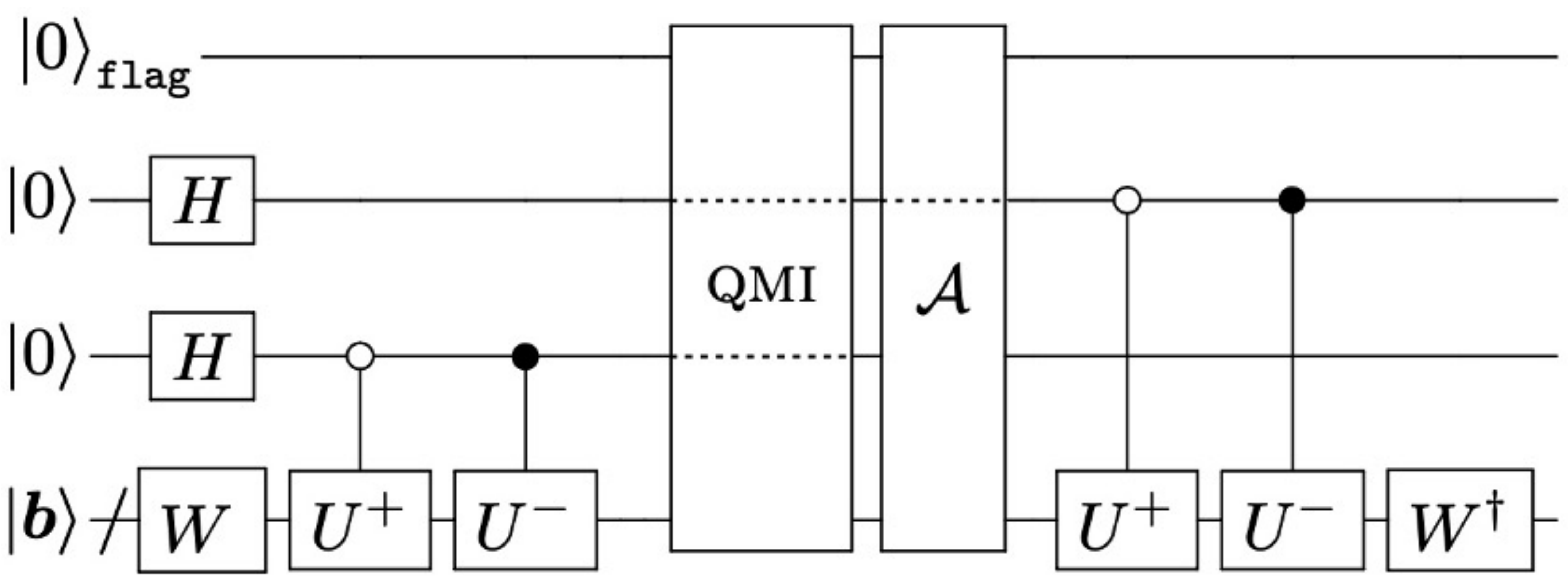
Generalization to PDEs

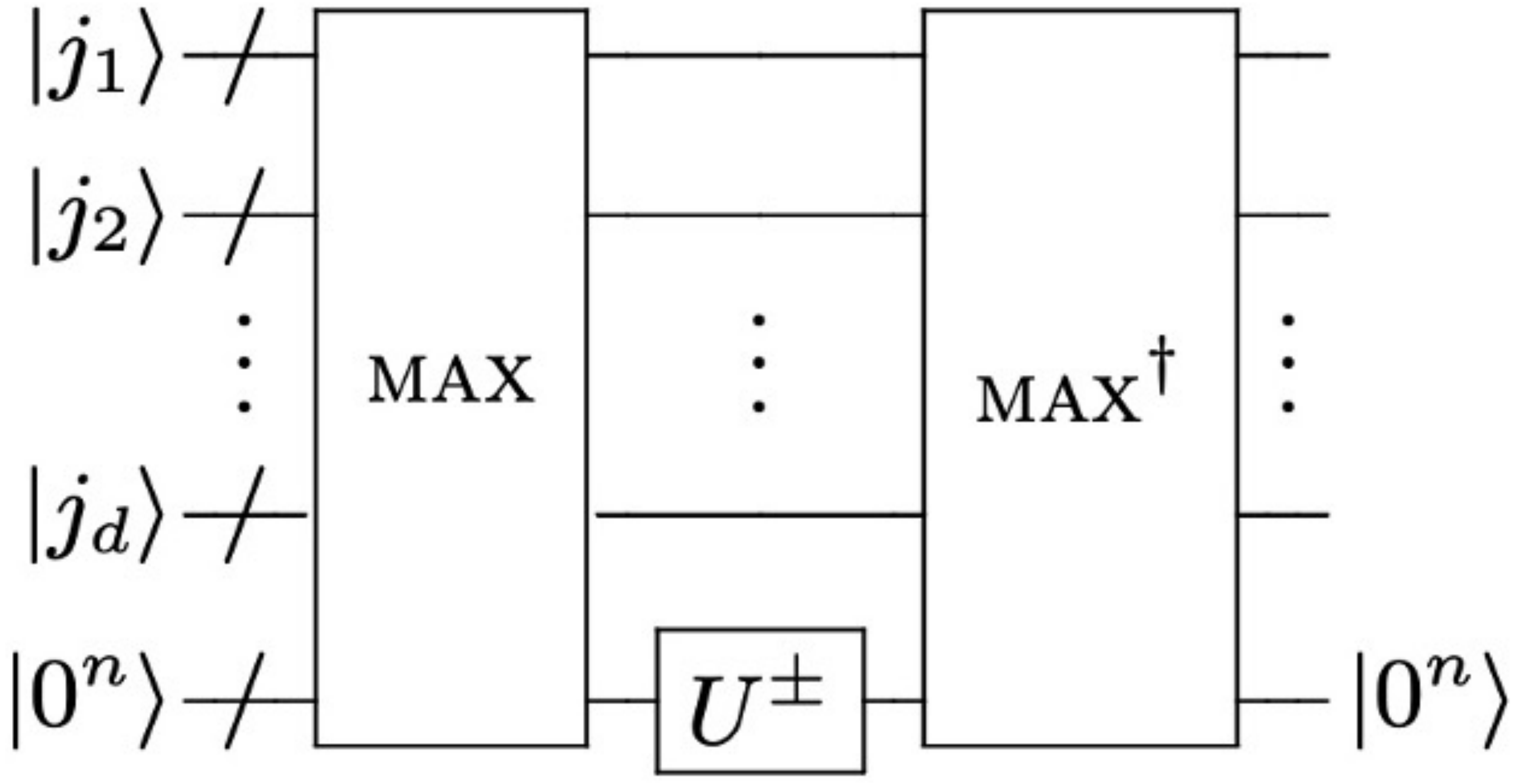
$$W \rightarrow W_{\mathrm{dD}} \coloneqq W \otimes W \otimes \cdots \otimes W$$

Cost: $\mathcal{O}(dn^2)$

$$U^{\pm} \rightarrow U^{\pm}_{\mathrm{dD}} \coloneqq \frac{1}{2}\left(P_{\mathrm{dD}} \pm \mathrm{i}\sqrt{\mathbb{I} - P^2_{\mathrm{dD}}}\right)$$

$$P_{\mathrm{dD}}|j_1\rangle|j_2\rangle\cdots|j_d\rangle \coloneqq 2^{-\lfloor j_{\max}\rfloor}|j_1\rangle|j_2\rangle\cdots|j_d\rangle$$

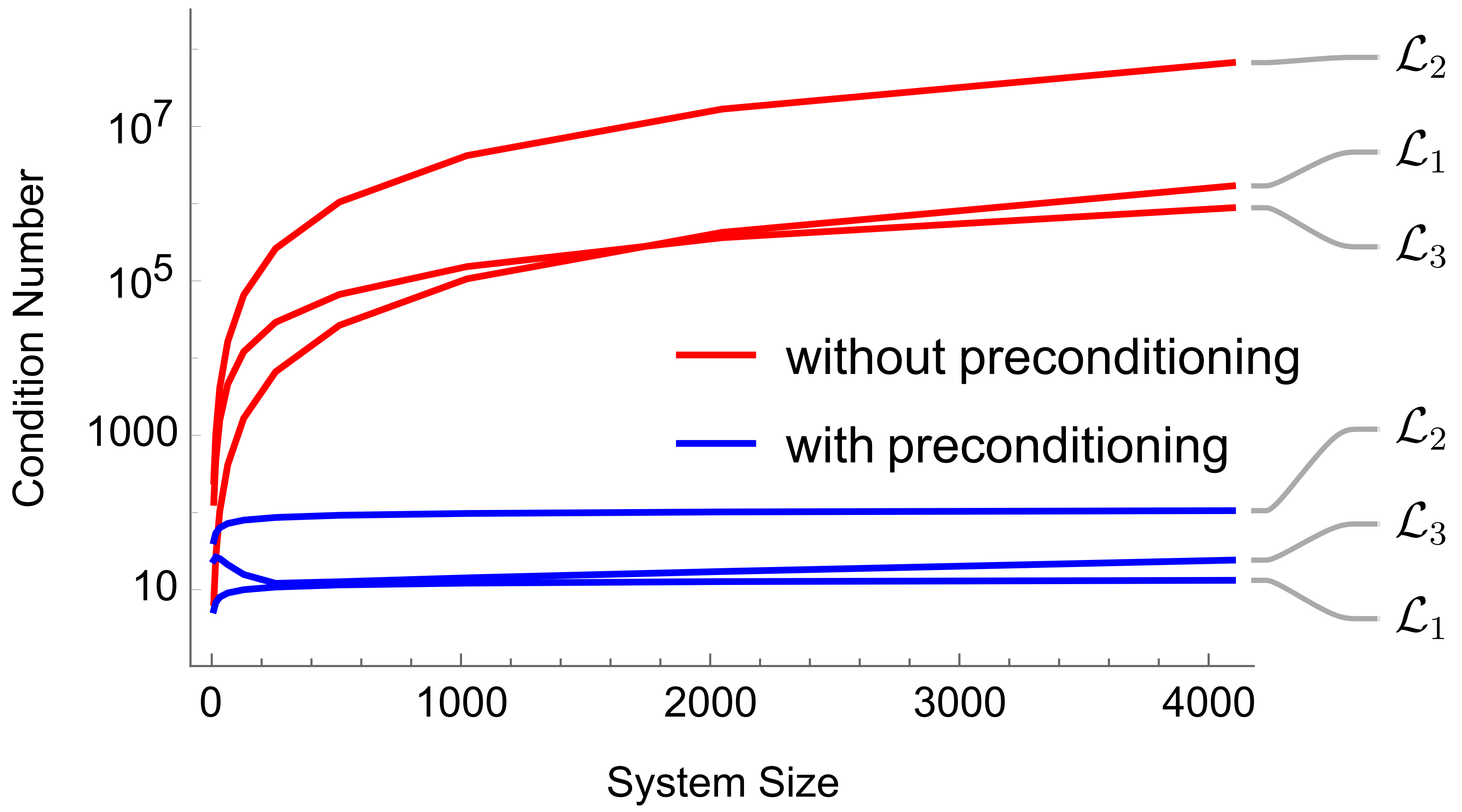




$\mathcal{O}(dn)$ $\mathcal{O}(n)$

Summary & Outlook

- Quantum algorithm with complexity in polylog(N), independent of κ.
- Class of fast-solvable PDEs.
- Optimally preconditionable in an auxiliary wavelet basis.



Limitations:

- The constant value for κ could be large for practical applications.
- Works for periodic boundary conditions.

Outlook:

- Hybrid approach $\longrightarrow$ Purely wavelet approach.
- Applications with fully fleshed out procedure.